Conformational Preferences of *N,N*-Dimethylsuccinamate as a Function of Alkali and Alkaline Earth Metal Salts: Experimental Studies in DMSO and Water as Determined by ^{1}H-NMR Spectroscopy

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Supporting Information

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Cartesian coordinates and ^{1}H-NMR spectra for *N,N*-dimethylsuccinamic acid (**1**) and its tetrabutylamonium salt (**1f**) can be found in the supporting information of:

Liu, A. T.; Emenike, B. U.; Carroll, W. R.; Roberts, J. D.; *Org. Lett.* **2013,** *15,* 760-763.

Cartesian Coordinates of *gauche*-**1a** B3LYP/6-31+G(2d,2p) Total Energy: -522.77960577 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.215712	1.101694	-0.913097
2	1	-0.408094	1.971616	-1.119525
3	1	0.747604	0.846406	-1.831080
4	6	1.281387	1.435732	0.172968
5	1	1.951637	2.197784	-0.229460
6	1	0.812362	1.804670	1.087175
7	6	2.027422	0.132200	0.449047
8	6	-0.611626	-0.135175	-0.575264
9	8	2.786248	-0.310041	-0.460870
10	8	-0.144631	-1.268966	-0.806762
11	7	-1.847795	-0.002489	-0.045643
12	6	-2.428025	1.244975	0.432943
13	1	-3.327329	1.496801	-0.139293
14	1	-2.709475	1.133928	1.484793
15	1	-1.721543	2.065657	0.362197
16	6	-2.640831	-1.194595	0.238846
17	1	-2.574353	-1.460813	1.299337
18	1	-3.686468	-0.993870	-0.008074
19	1	-2.275514	-2.025544	-0.358367
20	8	1.647611	-0.569896	1.428630
21	3	1.582561	-1.778991	-0.116280

Cartesian Coordinates of *trans*-**1a** B3LYP/6-31+G(2d,2p) Total Energy: -522.76885745 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.089123	-0.405129	-0.685384
2	1	0.169126	0.447607	-1.360160
3	1	0.404031	-1.284947	-1.246444
4	6	1.016566	-0.215277	0.523169
5	1	0.699028	0.629328	1.145953
6	1	0.980331	-1.091119	1.176938
7	6	2.472938	0.033784	0.168073
8	6	-1.343135	-0.689729	-0.247326
9	8	2.815752	0.247411	-1.038136
10	8	-1.711981	-1.849578	-0.088798
11	8	3.332421	0.034144	1.106109
12	7	-2.188640	0.368538	-0.017129
13	6	-3.554641	0.107415	0.410731
14	1	-3.730183	0.519077	1.411808
15	1	-4.263879	0.575194	-0.281625
16	1	-3.718013	-0.967160	0.429436
17	6	-1.839583	1.773621	-0.120873
18	1	-2.465420	2.272592	-0.871165
19	1	-2.002150	2.278479	0.839409
20	1	-0.799089	1.908182	-0.401042
21	3	4.503184	0.349689	-0.282317

Cartesian Coordinates of *gauche*-**1b** B3LYP/6-31+G(2d,2p) Total Energy: -677.409054 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.302054	-1.395297	0.068358
2	1	-0.986406	-2.142247	-0.340120
3	1	-0.226820	-1.573970	1.147544
4	6	1.088254	-1.591643	-0.554868
5	1	1.416276	-2.609312	-0.318877
6	1	1.051234	-1.498169	-1.641799
7	6	2.113485	-0.592006	-0.005394
8	6	-0.902111	0.001044	-0.102610
9	8	2.067603	-0.344843	1.233640
10	8	-0.205831	1.008104	-0.297718
11	7	-2.257024	0.115031	-0.015652
12	6	-3.161232	-0.977954	0.321018
13	1	-3.984044	-0.578115	0.918885
14	1	-3.587186	-1.445554	-0.574878
15	1	-2.663322	-1.739317	0.916005
16	6	-2.895815	1.403835	-0.250558
17	1	-3.737176	1.274979	-0.938194
18	1	-3.274893	1.830243	0.685279
19	1	-2.173643	2.088574	-0.686829
20	8	2.835260	0.023601	-0.835969
21	11	1.885975	1.727718	0.298841

Cartesian Coordinates of *trans*-**1b** B3LYP/6-31+G(2d,2p) Total Energy: -677.406866 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.366032	-0.444606	-0.686940
2	1	-0.221023	0.431209	-1.319725
3	1	-0.078026	-1.315039	-1.277093
4	6	0.536367	-0.348970	0.552748
5	1	0.213788	0.464345	1.214161
6	1	0.469475	-1.261383	1.149890
7	6	2.011119	-0.091080	0.243762
8	6	-1.823406	-0.673165	-0.306885
9	8	2.336276	0.344944	-0.901920
10	8	-2.270003	-1.815057	-0.243349
11	8	2.844574	-0.309877	1.173399
12	7	-2.610026	0.417699	-0.018698
13	6	-3.992160	0.212151	0.384475
14	1	-4.152131	0.569796	1.408976
15	1	-4.667444	0.763583	-0.279919
16	1	-4.218654	-0.849985	0.334198
17	6	-2.170849	1.800713	-0.011656
18	1	-2.794991	2.402023	-0.684079
19	1	-2.256297	2.228393	0.995579
20	1	-1.138115	1.893342	-0.333902
21	11	4.423326	0.296316	-0.214114

Cartesian Coordinates of *gauche*-**1c** B3LYP/6-31+G(2d,2p) Total Energy: -1115.023896 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.715842	-1.534916	-0.028789
2	1	-1.468354	-2.193981	-0.474219
3	1	-0.723903	-1.713178	1.052055
4	6	0.671370	-1.886837	-0.569837
5	1	0.855878	-2.947875	-0.367873
6	1	0.723950	-1.750055	-1.651566
7	6	1.796423	-1.064486	0.080882
8	6	-1.129466	-0.081725	-0.254128
9	8	1.630157	-0.705340	1.280731
10	8	-0.334679	0.779869	-0.649783
11	7	-2.431943	0.244397	-0.000401
12	6	-3.428417	-0.669007	0.538303
13	1	-4.000139	-0.157545	1.319042
14	1	-4.131611	-0.996902	-0.237432
15	1	-2.965486	-1.543786	0.985038
16	6	-2.913569	1.590187	-0.273518
17	1	-3.832519	1.540805	-0.866928
18	1	-3.134927	2.124251	0.658257
19	1	-2.155069	2.136715	-0.827851
20	8	2.759407	-0.721428	-0.655431
21	19	2.091248	1.623508	0.192246

Cartesian Coordinates of *trans*-**1c** B3LYP/6-31+G(2d,2p) Total Energy: -1115.021279 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.807404	-0.525345	-0.687287
2	1	-0.573984	0.369222	-1.265766
3	1	-0.568833	-1.388020	-1.311123
4	6	0.066929	-0.552219	0.578748
5	1	-0.280549	0.199116	1.298890
6	1	-0.004412	-1.518835	1.080063
7	6	1.544873	-0.238131	0.312988
8	6	-2.290409	-0.650461	-0.369369
9	8	1.822746	0.595473	-0.601045
10	8	-2.847563	-1.743562	-0.423490
11	8	2.402841	-0.808328	1.046671
12	7	-2.979141	0.483539	-0.004002
13	6	-4.385410	0.380186	0.349566
14	1	-4.541730	0.662842	1.397991
15	1	-4.985425	1.049721	-0.277860
16	1	-4.710589	-0.646626	0.200952
17	6	-2.411296	1.812951	0.125730
18	1	-2.960219	2.523122	-0.505139
19	1	-2.482645	2.164028	1.163440
20	1	-1.366297	1.833393	-0.169165
21	19	4.315830	0.297722	-0.190717

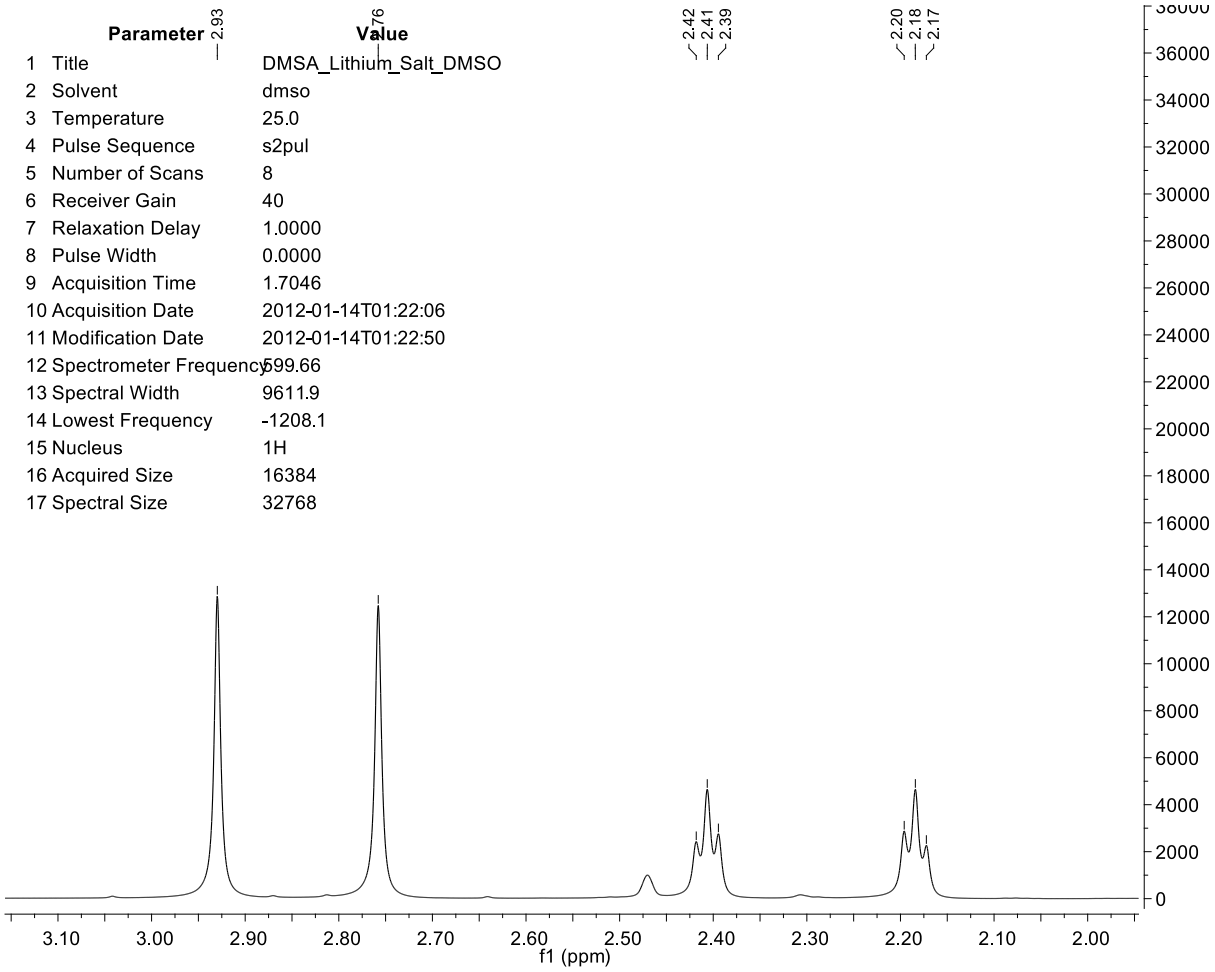
Cartesian Coordinates of *gauche*-**1d** B3LYP/6-31+G(2d,2p) Total Energy: -1230.318010 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.889733	-2.220281	-0.567914
2	1	3.220583	-2.581138	0.407463
3	1	3.097038	-2.972498	-1.331135
4	6	3.623092	-0.902684	-0.962968
5	1	3.355162	-0.673673	-1.996147
6	1	4.701820	-1.042920	-0.921160
7	6	1.415442	-1.862541	-0.525594
8	6	3.142416	0.302228	-0.156862
9	8	0.837527	-1.590952	-1.618577
10	8	2.028641	0.793569	-0.408880
11	7	3.922597	0.841394	0.808999
12	6	3.456779	2.019937	1.536170
13	1	2.538619	2.383575	1.083817
14	1	4.224917	2.798695	1.500085
15	1	3.265075	1.764393	2.583241
16	6	5.202248	0.315543	1.261049
17	1	5.398480	-0.670792	0.852777
18	1	5.189528	0.230376	2.351857
19	1	6.021783	0.987175	0.980816
20	8	0.894520	-1.579635	0.592362
21	1	-3.220448	2.581155	0.407595
22	6	-2.889666	2.220277	-0.567799
23	1	-3.097002	2.972495	-1.331012
24	6	-3.623109	0.902710	-0.962790
25	1	-4.701828	1.043003	-0.920901
26	1	-3.355260	0.673664	-1.995984
27	6	-3.142420	-0.302190	-0.156681
28	6	-1.415371	1.862535	-0.525569
29	8	-2.028628	-0.793488	-0.408689
30	8	-0.894338	1.579744	0.592360
31	7	-3.922646	-0.841391	0.809125
32	6	-3.456865	-2.019937	1.536318
33	1	-3.265298	-1.764414	2.583419
34	1	-2.538638	-2.383527	1.084066
35	1	-4.224964	-2.798729	1.500121
36	6	-5.202411	-0.315642	1.260964
37	1	-5.189931	-0.230646	2.351787
38	1	-6.021879	-0.987237	0.980443
39	1	-5.398556	0.670759	0.852802
40	8	-0.837558	1.590859	-1.618589
41	12	0.000052	-0.000020	-0.533388

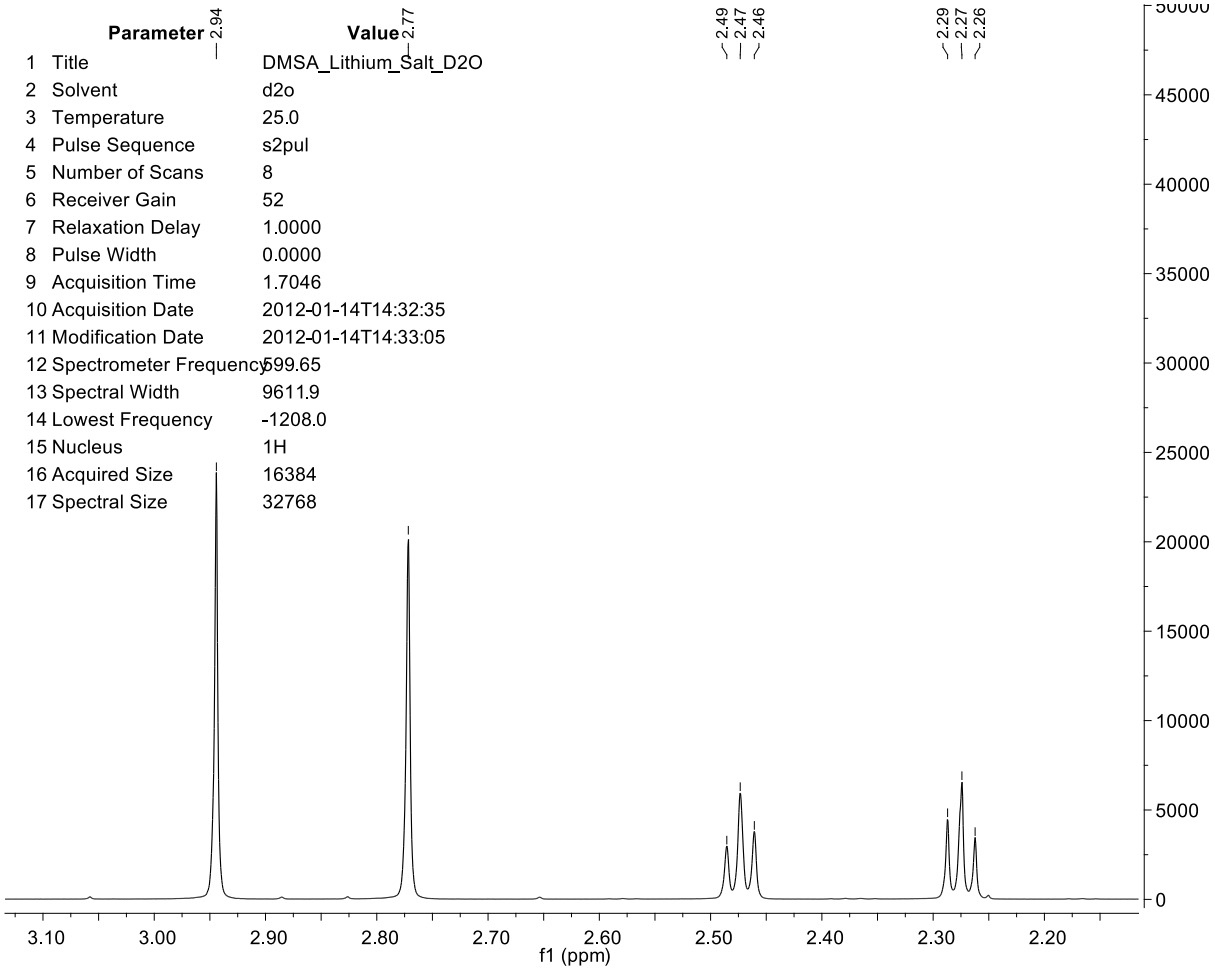
Cartesian Coordinates of *gauche*-**1e** B3LYP/6-31+G(2d,2p) Total Energy: -1707.827606 au

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.659759	-0.920925	-1.487172
2	1	4.472892	-1.204453	-0.816316
3	1	3.930265	-1.168858	-2.515268
4	6	3.379459	0.608119	-1.409558
5	1	2.660864	0.860947	-2.190346
6	1	4.292966	1.172967	-1.599682
7	6	2.375362	-1.634311	-1.074468
8	6	2.706423	1.007496	-0.101605
9	8	2.258486	-1.973668	0.138427
10	8	1.465978	0.922525	-0.012577
11	7	3.442084	1.444623	0.943698
12	6	2.777283	1.790547	2.197519
13	1	1.720739	1.964594	2.014406
14	1	3.237163	2.692835	2.609218
15	1	2.882078	0.978069	2.924374
16	6	4.896099	1.418811	1.013944
17	1	5.216384	0.735018	1.806992
18	1	5.280233	2.417715	1.244600
19	1	5.334655	1.082618	0.079982
20	8	1.419056	-1.660547	-1.900232
21	1	-4.183447	-1.929665	1.744277
22	6	-3.617423	-1.053531	1.421207
23	1	-3.880950	-0.198760	2.047306
24	6	-3.953841	-0.783285	-0.072460
25	1	-3.751597	-1.697884	-0.632230
26	1	-5.011821	-0.547662	-0.189522
27	6	-3.050466	0.275518	-0.692088
28	6	-2.117149	-1.322985	1.508221
29	8	-1.917201	-0.050170	-1.093227
30	8	-1.361742	-0.381983	1.885161
31	7	-3.477551	1.552666	-0.812892
32	6	-2.610649	2.545316	-1.441276
33	1	-1.858734	2.042264	-2.043024
34	1	-2.108930	3.156852	-0.683727
35	1	-3.217016	3.197449	-2.075349
36	6	-4.702433	2.087868	-0.235044
37	1	-4.458375	2.937839	0.410030
38	1	-5.214459	1.346474	0.369910
39	1	-5.380145	2.436901	-1.021628
40	8	-1.689138	-2.401104	1.005732
41	20	0.021373	-1.050426	-0.017461

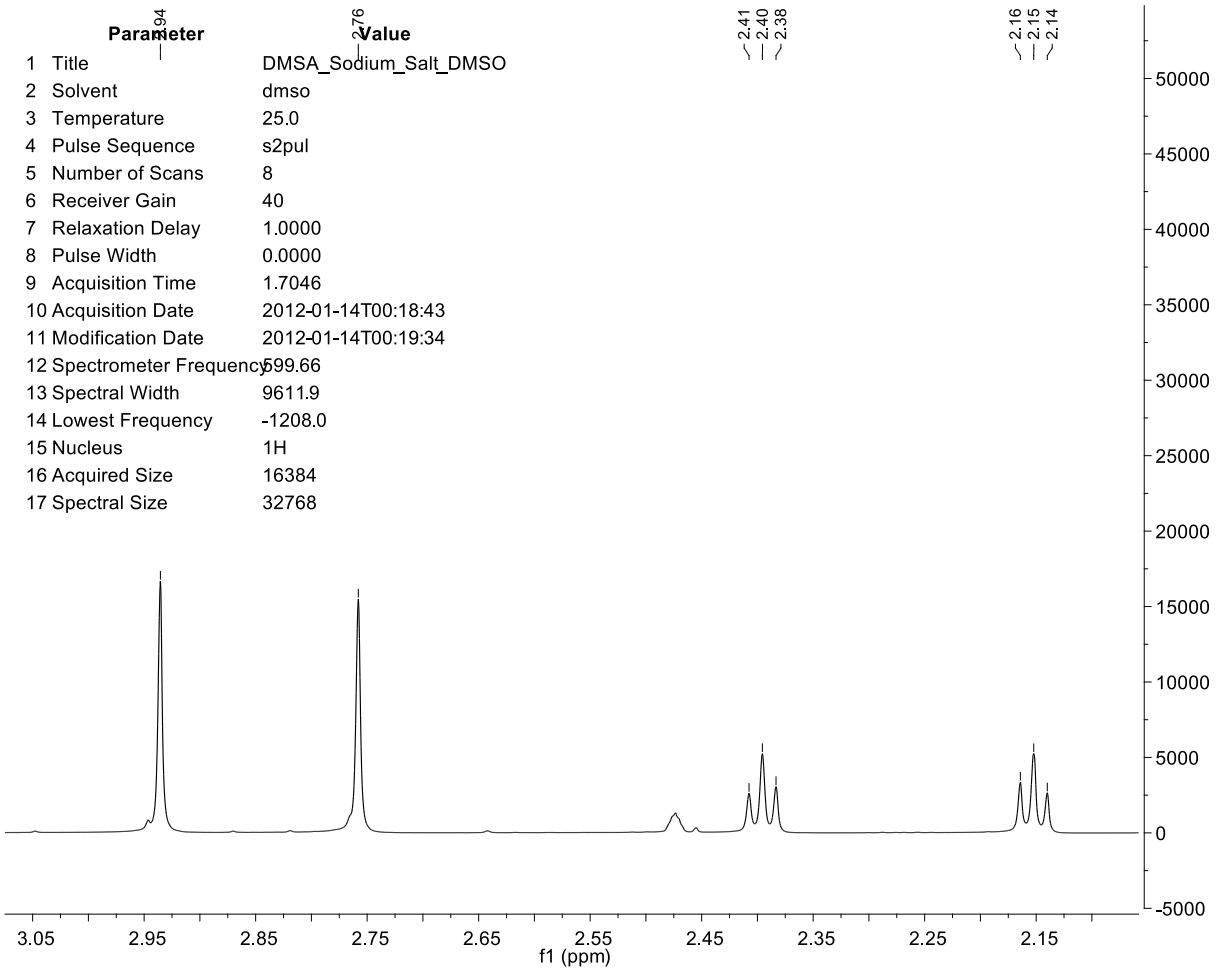
Lithium *N,N*-dimethylsuccinamate (**1a**) in DMSO



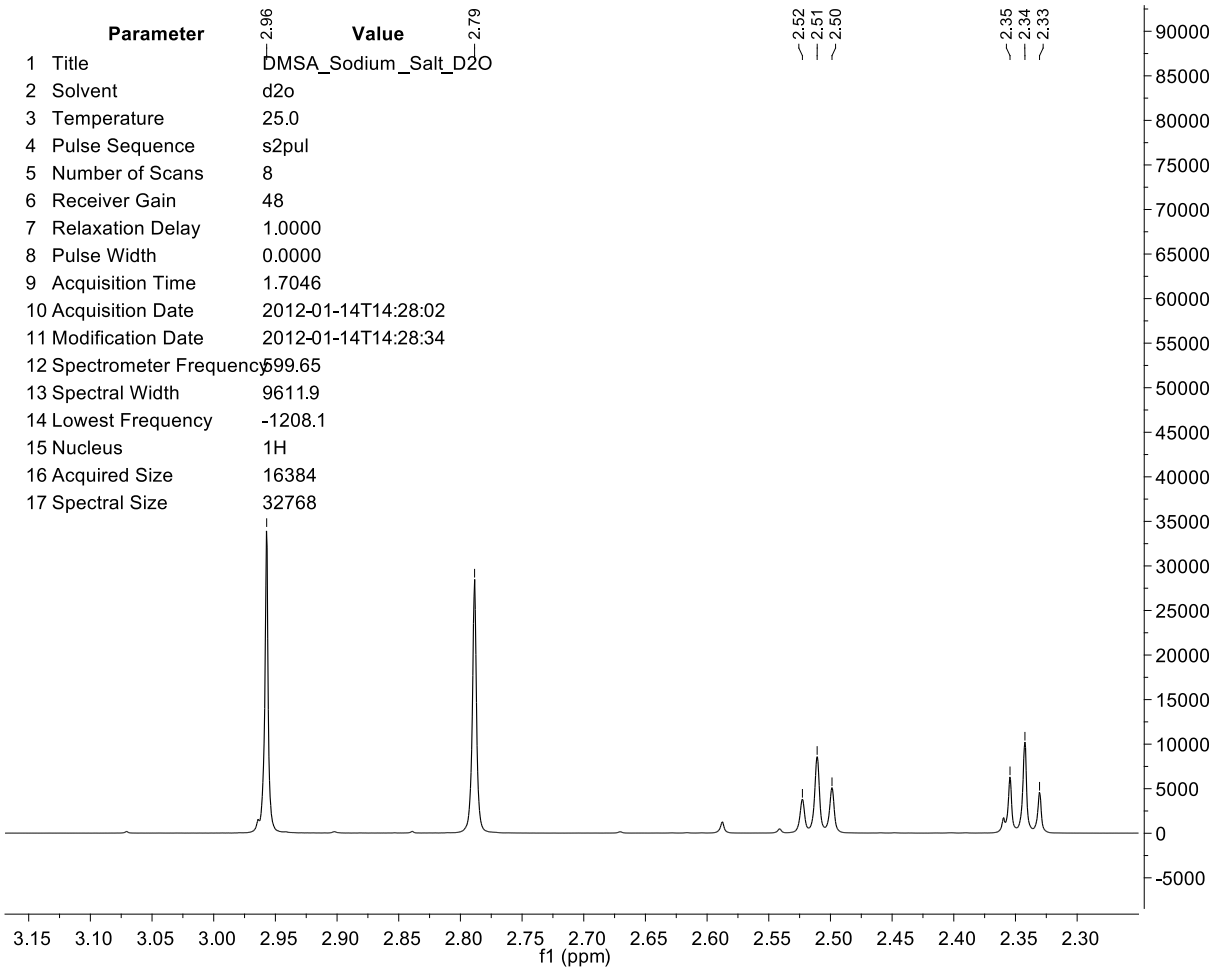
Lithium *N,N*-dimethylsuccinamate (**1a**) in D_2O



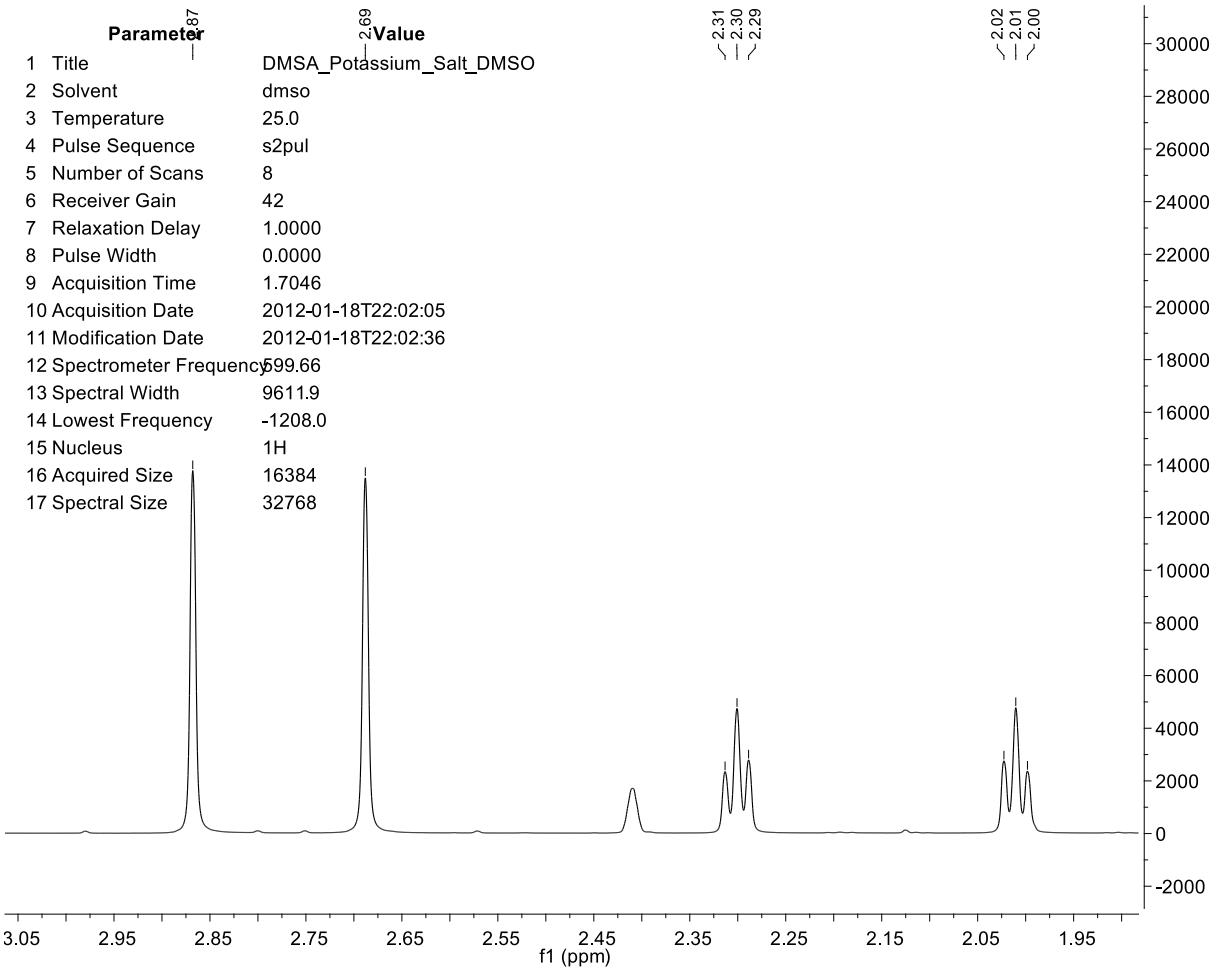
Sodium *N,N*-dimethylsuccinamate (**1b**) in DMSO



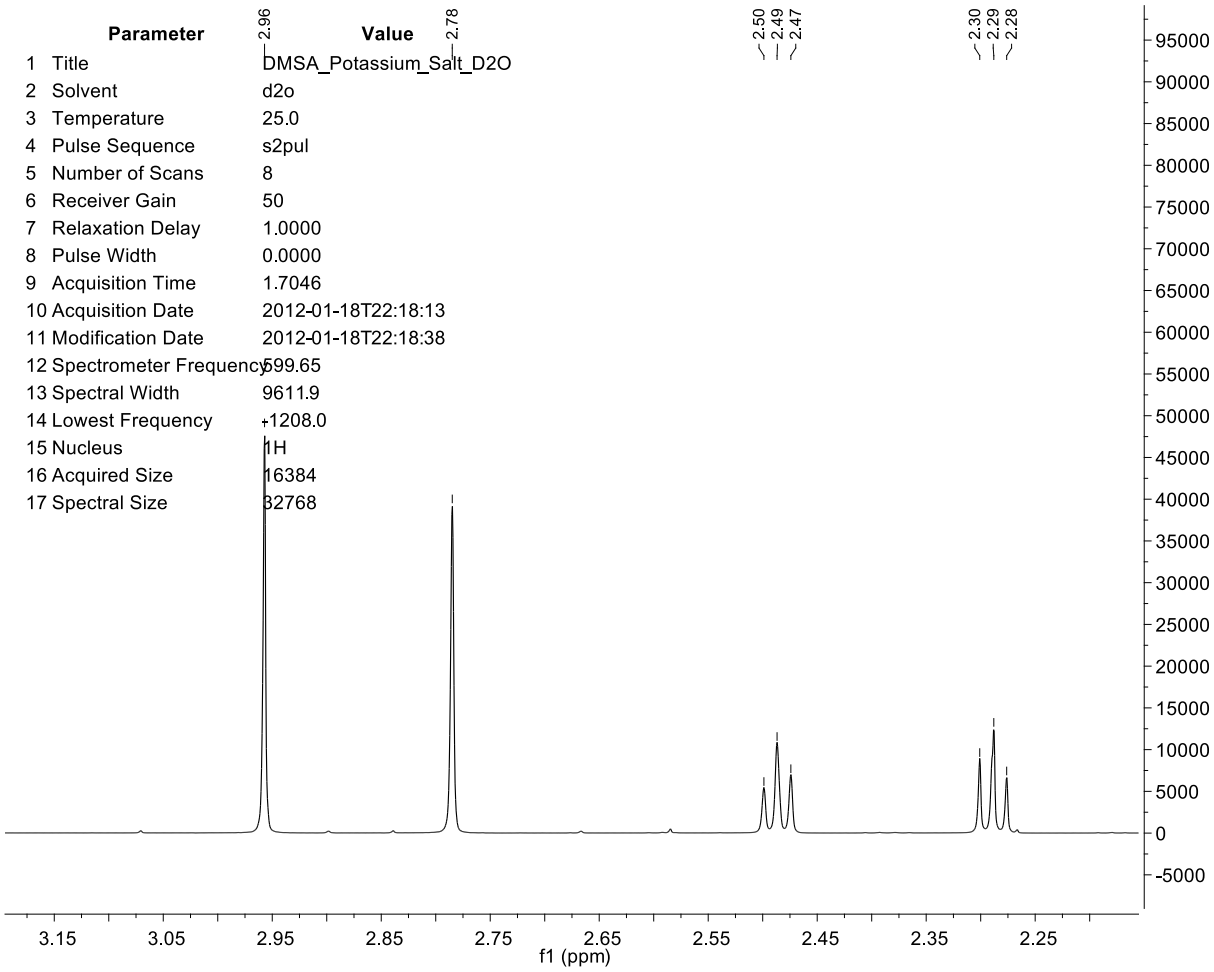
Sodium *N,N*-dimethylsuccinamate (**1b**) in D_2O



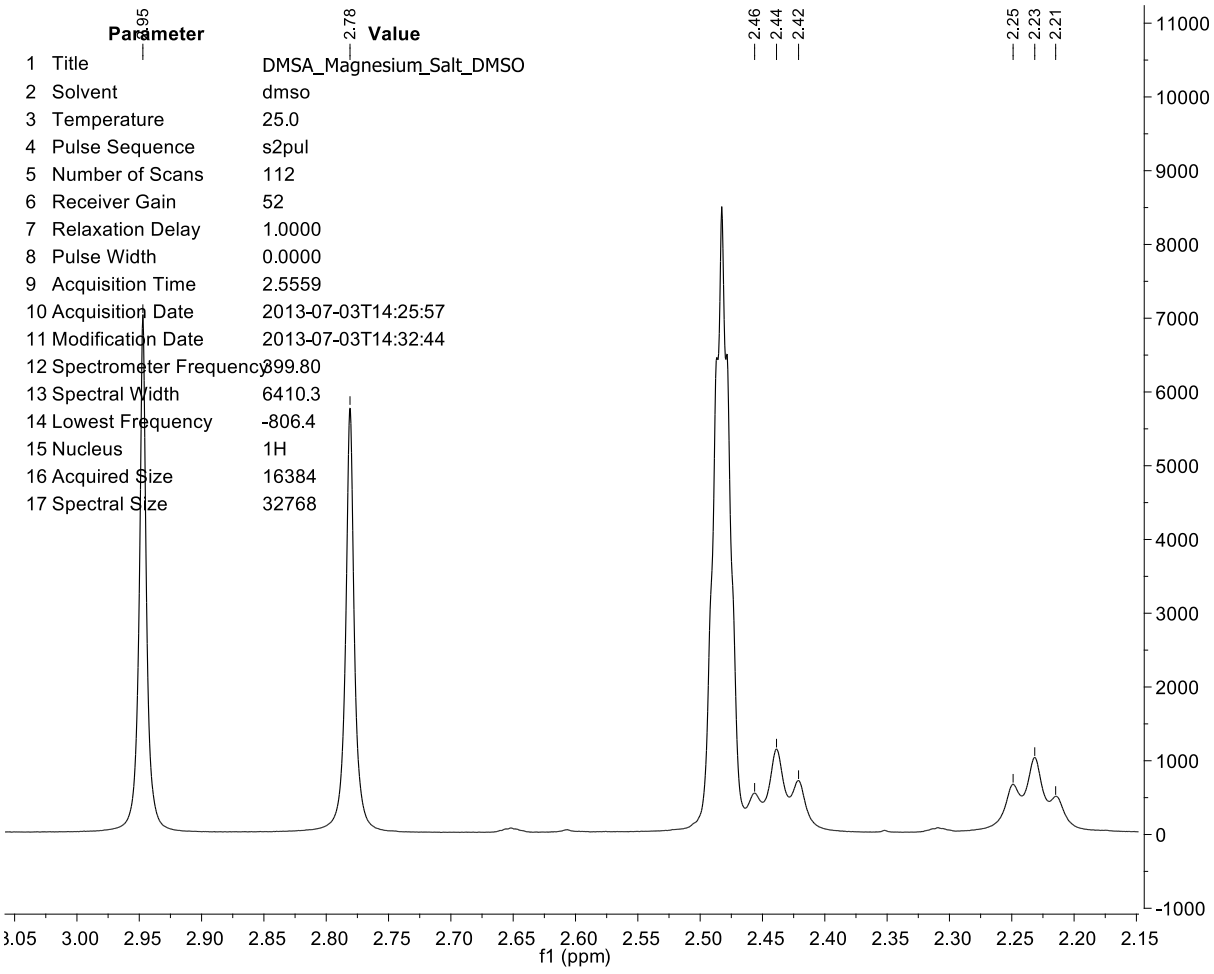
Potassium *N,N*-dimethylsuccinamate (**1c**) in DMSO



Potassium *N,N*-dimethylsuccinamate (**1c**) in D_1O



Magnesium *N,N*-dimethylsuccinamate (**1d**) in DMSO



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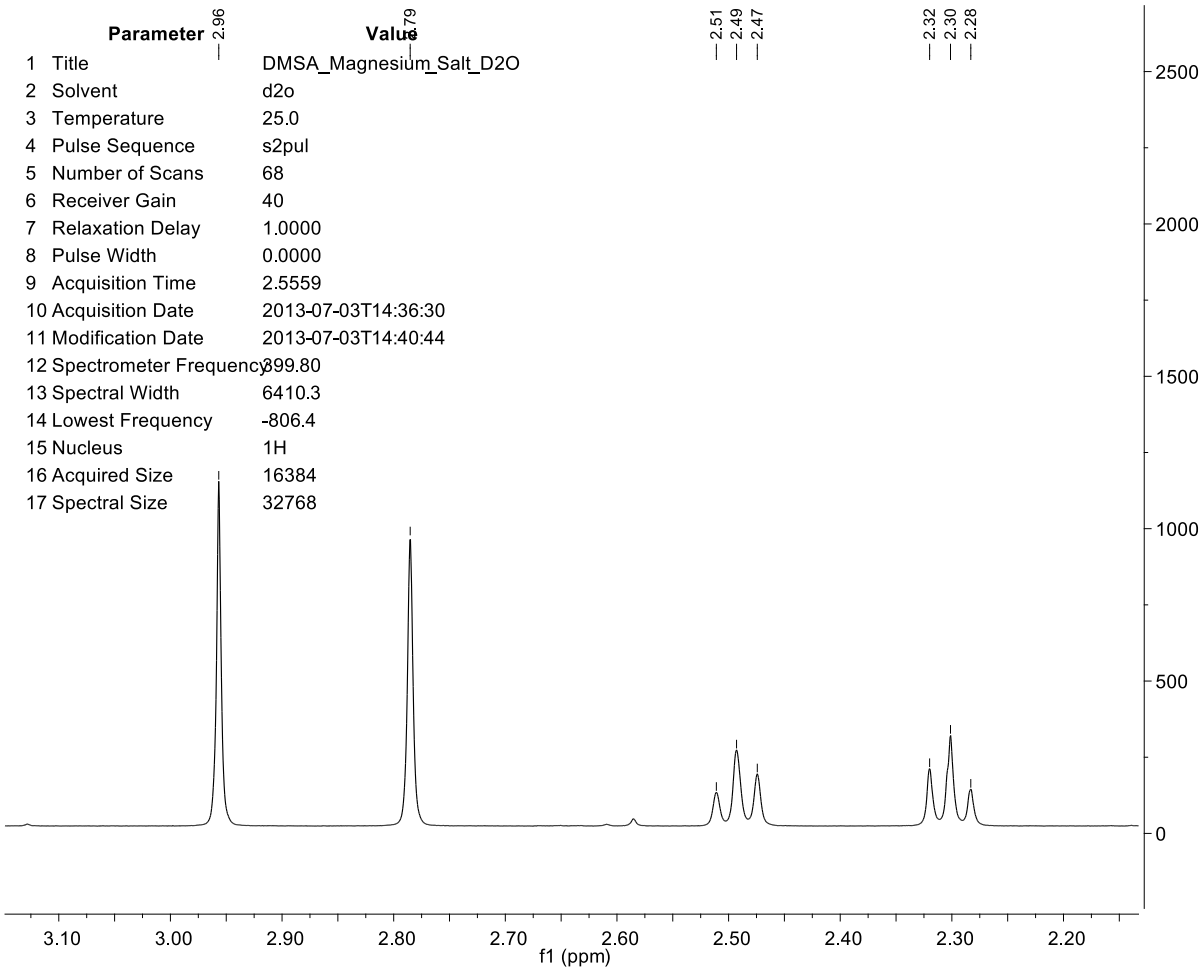
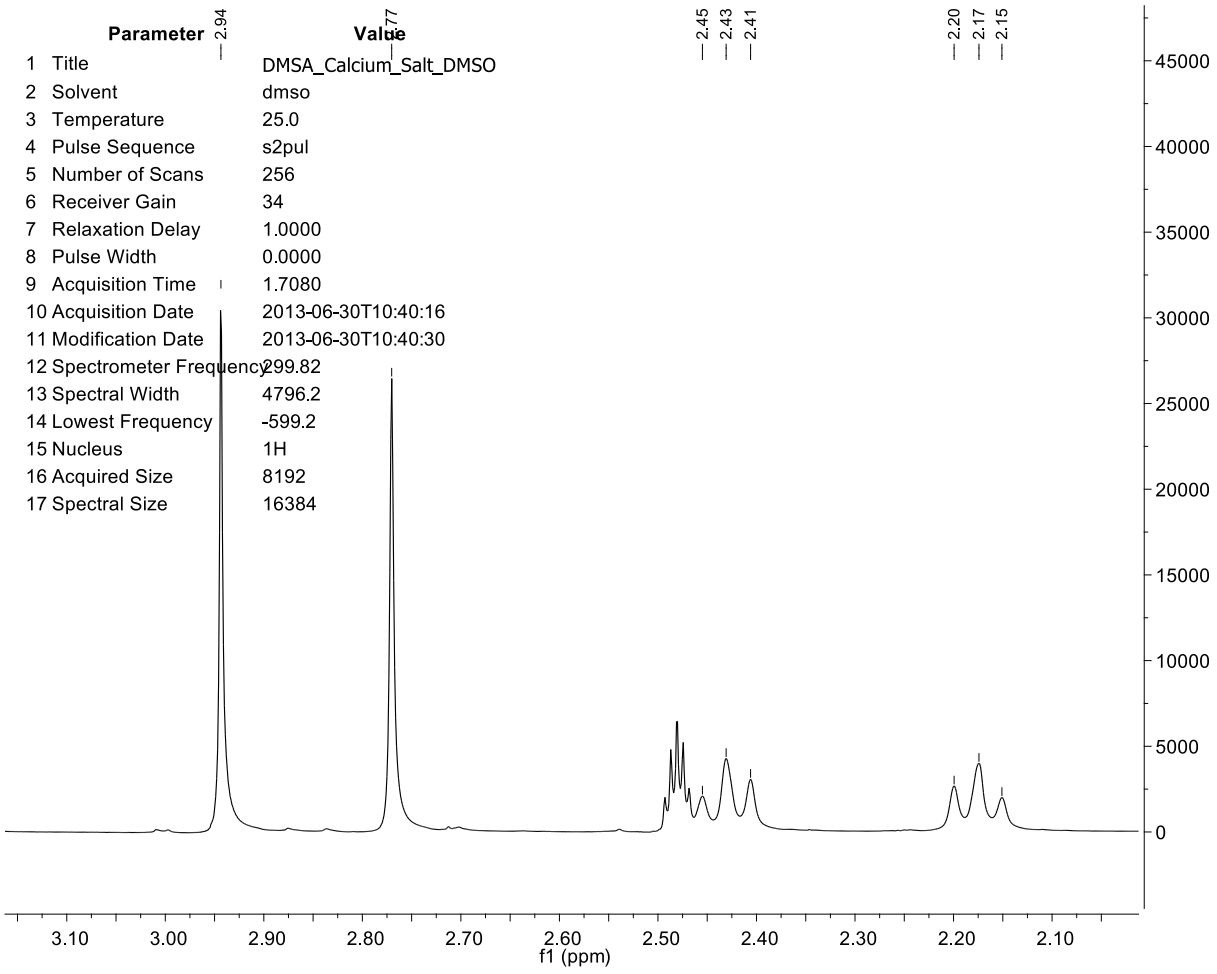
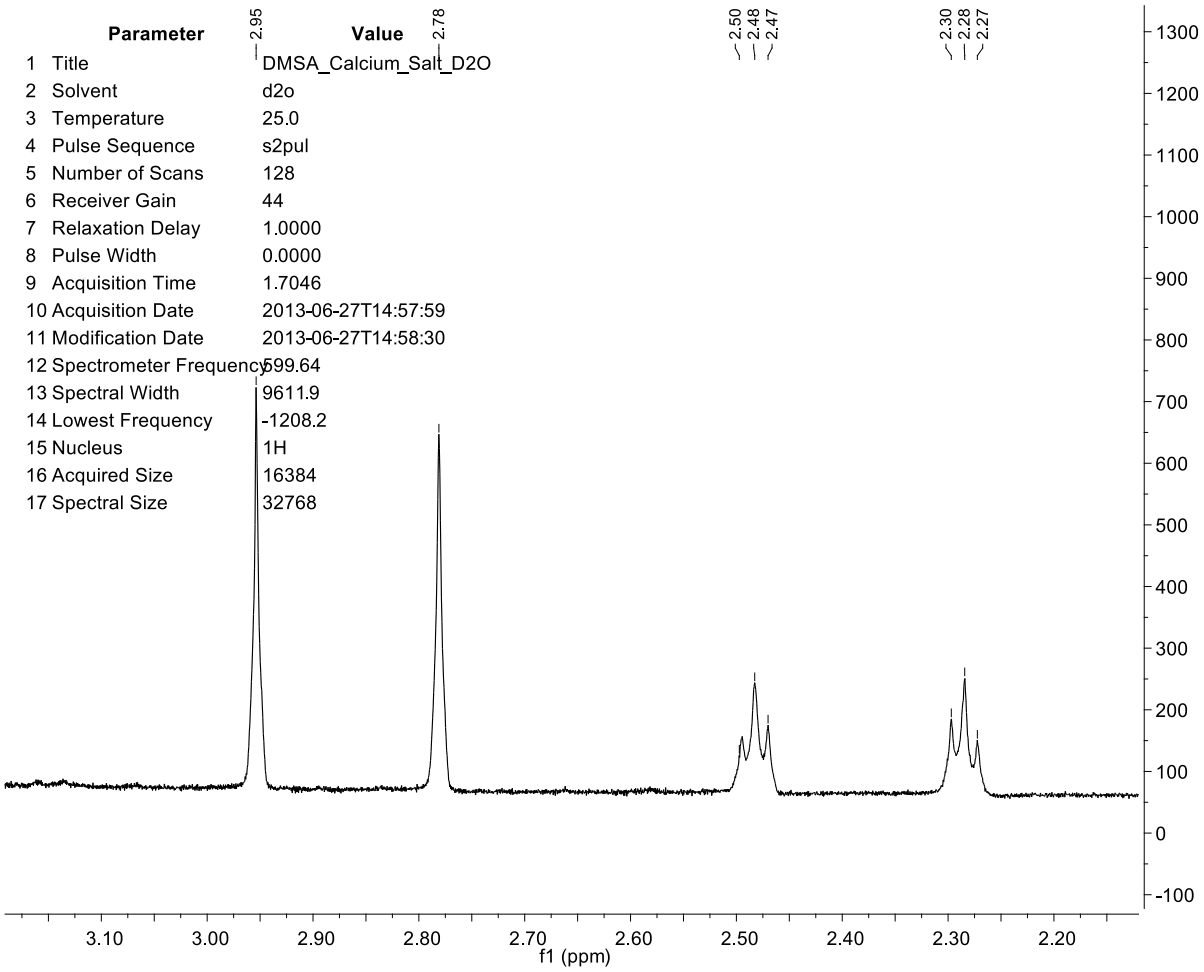


Calcium *N,N*-dimethylsuccinamate (**1e**) in DMSO



Calcium *N,N*-dimethylsuccinamate (**1e**) in D_2O



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16 Acquired Size	16384
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